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# Simulation of Thin-Film Solar Cells based on (CCZTSe) Using (SCAPS-1D) Program

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**ABSTRACT**

This paper presents results of a computer-simulation study of a Thin-film solar-cell based on p-type CCZTSe-absorbent-layer and n-type CdS-buffer-layer in a structure of ($WS_2$+CCZTSe+CdS+ITO) using the simulation software (SCAPS-1D). The thickness of the absorbing layer made variable in the range (0.25-3μm), and one type of defect was added to the absorbent-layer in order to make the cell closer to practical reality. It was found that changing the thickness of the (CCZTSe)- layer results in an increase in the conversion-efficiency (η), from 23.27 - 26.66% with a maximum of 26.94% at a thickness of 1.25 μm, and an increase in short-circuit current density ($J_{SC}$) from 44 to 51.4 mA/cm$^2$. The fill-factor (FF), and the open-circuit voltage ($V_{OC}$) remains almost constant at about 83% and 0.63 V respectively. Increasing the defects- density ($N_{def}$ ) from 1E13 -to – 1E17 cm$^{-3}$, leads to a decrease in the efficiency from 27.27% to 13%. The FF decreases from 83.5% to about 70%, the short-circuit current density ($J_{SC}$) decreases from 51 - 41 mA/cm$^2$. the open-circuit voltage ($V_{OC}$) decreases from about 0.64 V to about 0.45 V. And we notice an improvement in efficiency (η), (FF), and ($V_{OC}$) when increasing the concentration of the acceptors ($N_A$) in the (CCZTSe)- absorption layer in the range (1E14-1E20cm$^{-3}$). The efficiency (η), increases from about 19.7% to about 27.6%, FF increases from 72- 83.6% and ($V_{OC}$) increases from 0.53 - 0.64 V, while ($J_{SC}$) remains almost constant. No change produced when we changed the donor-density ($N_D$) in the CdS buffer layer.

**Keywords**: SCAPS-1D, CCZTSe, Back surface Layer (BSL), solar cell, CdS buffer layer

## Introduction:

The need for energy is in rise worldwide, making energy production one of the world's most pressing challenges. Solar energy (SE) is used as a substitute for fossil fuels. It can be harnessed through a variety of methods, and it is environmentally acceptable [1]. Solar cells are important because they can convert a considerable quantity of sunlight directly into electrical energy [2]. To achieve high efficiency and cheap cost, a Thin-Film (CCZTSe)-cell is suggested in this study. Alloying different proportions of Cu2ZnSnSe4 (CZTS) and Cu2CdSnSe4 (CCTS) allows a variation in energy gap of (1.05-1.5 eV) [3]. However, contaminants may result in a reduction in cell conversion- efficiency [4]. Extending the wavelength of spectral absorption into the infrared is desirable. Yuying Jiao et al. used (SCAPS-1D) software to simulate an experimentally developed photovoltaic cell employing (ZNO) as the window layer, (CCZTSe) as the absorption layer, and (CdS) as the buffer layer in 2021. The study revealed that the CCZTSe layer is a promising material for infrared radiation detection [5]. Using the same computer program (SCAPS-1D), the present researchers hope to construct a high-efficiency photovoltaic cell by varying the thickness of the absorber layer, the density of flaws, and investigate their impact on the solar cell's performance.

Incident Light

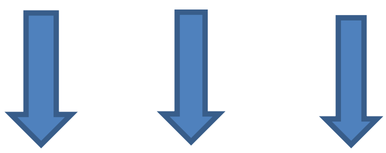

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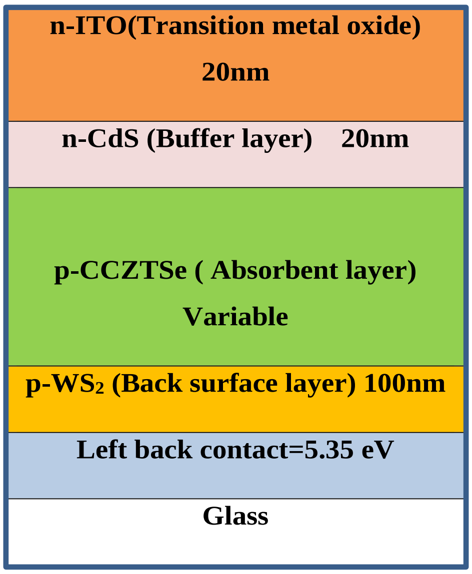
**Figure (1) Solar cell installation construction $WS_2$+CCZTSe+CdS+ITO**




**Numerical Modeling and Material Parameters:**

Photovoltaic devices may be studied using computer simulations, which have shown to be a viable method for determining the optical, electrical, and mechanical characteristics of complicated photovoltaic devices. PV device manufacturing costs and researcher time can be reduced by offering a set of helpful guidelines for adjusting production settings to improve device performance. In recent years, numerical modeling has emerged as a significant tool for building and simulating efficient solar cells [6]. SCAPS-1D, is a one-dimensional computer simulation tool created by Ghent University's Electronics and Information Systems (ELIS). The software is open source and may be used for a wide range of solar research projects. The SCAPS software relies on the Poisson equation and the electron-hole equations. I-V, C-V, C-f, and QE characteristics can be obtained from the simulation. In order to model and create the solar cell shown in Figure 1, the (SCAPS-1D) software was employed. Measurements were taken at a temperature of( 300 K). Equations 1- 5 (given below) were used to derive values of ($V_{OC}$, $J_{SC}$, FF, efficiency-Ƞ and Quantum efficiency QE) [7].

The Open-Circuit-Voltage ($V_{OC}$) when the load resistance is infinite is given by Equation (1). It is obvious that $V_{OC}$ depends on $I_L$ (light-generated current or photovoltaic-current) and the saturation-current $I_0$ [8].

$$V_{OC} = \frac{nKT}{q} \ln(\frac{I_L}{I_0} + 1) \qquad \text{at } I=0 \qquad \text{--------------(1)}$$

The short-circuit-current density ($J_{SC}$) is defined as the greatest output current-density when the cell is short circuited.

$$J_{SC}(V) = J_O \left(e^{qV/nk_BT} - 1\right) \qquad \text{---------------------(2)}$$

Where ($J_0$) is the saturation-current-density. There are several factors that affect the short circuit current, the intensity of lamination, cell optical properties and p-n junction thickness [9].

The Fill-Factor (FF) of the cell is given by:

$$FF = \frac{V_{mp} \cdot J_{mp}}{J_{OC}\, V_{OC}} \qquad \text{------------------------(3)}$$

The FF is usually in the range of (0.70 - 0.85 %).

The conversion-efficiency (η) is given by:

$$\eta = \frac{P_{mp}}{P_{in}} = \frac{V_{OC}\, J_{SC}\, FF}{P_{in}} \qquad \text{--------- -------------(4)}$$

The conversion-efficiency (η) is the output electrical-power divided by input optical-power (the product of solar radiation intensity with the cell area).

The quantum-efficiency (QE) is given by:

$$QE = \frac{hcR_\lambda}{q\lambda}$$

hc/q=1.24 is a constant value, hence:

$$QE = 1.24\left(\frac{R_\lambda}{\lambda}\right) \qquad \text{------------------ (5)}$$

$R_\lambda$: is the spectral-response in units (A/W), λ is the wavelength (nm)

Quantum efficiency (QE) may be defined as the number of electron-hole -pairs created by each photon landing on the absorbing layer, which is a significant characteristic in photovoltaic applications.

The simulation program sets the global default light spectrum at 1.5AM with a light intensity of 1000 ($W/m^2$) [10]. The cell (see Figure 1) consists from a transparent layer of transition-metal oxide (ITO), an n-type cadmium-sulfide (CdS) buffer semiconductor layer with a large energy gap and a high refractive index that produces the necessary n-p junction with the next p-type CCZTSe absorbing layer.The next layer is a p-type tungsten-disulfide $WS_2$ material which is the layer responsible for returning electrons to improve cell performance [11]. The n-p junction is formed between the CdS and the absorbing layer [12].

**Results and Discussion:**

**1- Effect of changing the thickness of the absorbent layer**

Table (1) displays the main parameters of the cell (see Figure 1). To study the influence of absorber layer thickness on the performance, the thickness of the absorbing layer (p-CCZTSe) was changed from 0.25- 3μm. The concentration of defects density ($N_{def}$) initially is kept constant at (1E14 $cm^{-3}$). The thickness of the BSL layer, the window layer, and the buffer layer was kept constant at (0.1 μm), (0.02 μm) and (0.02 μm) respectively. In the model we assumed a fixed interface-defects in the CCZTSe/CdS junction at 1E15 $cm^{-3}$. Table (2) shows the concentration of interface defects and the associated capture cross-sections. When the thickness of the absorbent layer increases the absorption of photons increases and thus lead to an increase in the properties of the cell [11]. We add defects in the range from 1E13 - 1E17 $cm^{-3}$ to the absorption layer to bring the simulation-model closer to practical reality [13] and to determine the effect of this addition on the properties. We add one type of defects to make the model as simple as possible. Defects are added to increase the electrical conductivity or control of cell performance, but high concentration of defects may reduce the conversion-efficiency [14].Figure (3) shows increase in short circuit current density ($J_{SC}$) from (44 $mA/cm^2$) at thickness (0.25 μm) to (51 $mA/cm^2$) at thickness (3μm). Open circuit voltage ($V_{OC}$) generally decreases slightly with increasing thickness from (0.633V) at thickness (0.25μm) to (0.624V) at thickness (3μm). When the concentration of defects is reduced, we notice an increase in the conversion efficiency due to the small number of interface defects and the increase in the homogeneity of the surface in the cell [15]. Figure (3) shows the quantum efficiency (QE) as a function of photon-wavelength with absorbent-layer thickness as a parameter. It is noted from Figure (3) that the quantum efficiency (QE) peaked with the increase in the thickness of the absorbing layer, and this means that the incident photons of different wavelengths were absorbed at different depths of the photovoltaic cell.

Figure (4) shows ($J_{SC}$) and ($V_{OC}$) as a function of thickness of the p-CCZTSe absorption layer. ($J_{SC}$) of the cell increases with the thickness of the (p-CCZTSe)- layer because the thicker absorbent layer will absorb more photons of longer wavelength, thus generating electron-hole pairs. The figure shows that ($V_{OC}$) decreases slightly from 0.635V -to- 0.624V with increasing thickness. Figure (5) shows the conversion-efficiency (η) increases with the increase in the thickness of the absorbent (p-CCZTSe)- layer, from about (23.3%) to about (26.7%) in the thickness range from (0.25μm) to (3μm). The increase in the efficiency may be attributed to the generation of voltage barrier between the back reflection layer and the absorbing layer. The back reflection layer returns the electrons and prevents their accumulation, thus reducing the recombination process, and increasing the cell efficiency [16]. The fill factor (FF) increases slightly from (83.35%) at 0.25μm thickness to up 83.38% at 1.25 μm then decreases slightly down to 83.03% at 3.0μm thickness as shown in Figure (5).

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**Table (1) The main parameters of the cell.**

| Parameter | Symbol (unit) | CCZTSe [5] | $WS_2$ [17] | CdS [18] | ITO [4] |
|---|---|---|---|---|---|
| **Thickness** | d (μm ) | Variable | 0.1 | 0.02 | 0.02 |
| **Band gap** | Eg (eV) | 0.9 | 1.29 | 2.4 | 3.6 |
| **Electron affinity** | χ (eV) | 4.4 | 4.05 | 4.2 | 4.1 |
| **Dielectric permittivity** | rϵ/ϵ | 10 | 13.6 | 10 | 10 |
| **CB effective density of states** | $(cm^{-3})N_C$ | 2.2 E+18 | 2.2E+18 | 2.2 E+18 | 2 E+18 |
| **VB effective density of states** | $(cm^{-3})N_V$ | 1.8 E+19 | 1.8 E+19 | 1.8 E+19 | 1.8E+19 |
| **Electron thermal velocity** | $(cm/s)V_n$ | 1.0 E+7 | 1.0 E+7 | 1.0 E+7 | 1.0 E+7 |
| **Hole thermal velocity** | $(cm/s)V_P$ | 1.0 E+7 | 1.0 E+7 | 1.0 E+7 | 1.0 E+7 |
| **Electron mobility** | $(cm^2/v.s)\mu_n$ | 60 | 100 | 100 | 50 |
| **Hole mobility** | $(cm^2/v.s)\mu_p$ | 20 | 100 | 25 | 75 |
| **donor density** | $N_D$ $(cm^{-3})$ | 0 | 0 | Variable | 1E18 |
| **acceptor density** | $N_A$ $(cm^{-3})$ | Variable | 1E18 | 0 | 0 |
| **Characteristic energy in a Gauss defect distribution** | $W_G$ ( eV) | 0.1 [19] | 0.1 [19] | 0.1 [19] | 0.1 [19] |
| **Defect Density** | $N_{def}$ $(cm^{-3})$ | (D) Variable | (D) 2E12 [19] | (D) 5E17 [20] | (D) 1E15 [19] |
| **Electron capture cross section** | $\sigma_e$ $(cm^2)$ | $10^{-15}$ [20] | $10^{-12}$ [19] | $10^{-15}$ [20] | $10^{-12}$ [19] |
| **Hole capture cross section** | $\sigma_h$ $(cm^2)$ | $10^{-15}$ [20] | $10^{-15}$ [19] | $10^{-15}$ [20] | $10^{-15}$ [19] |

**Table (2): - Interface Gaussian Defect States.**

| Parameters | Symbol (unit) | CCZTSe/CdS |
|---|---|---|
| **Gaussian defect density** | $N_t$ $(cm^{-3})$ | 1E15(D) |
| **Electron capture cross section** | $\sigma_e$ $(cm^2)$ | 1E-16 |
| **Hole capture cross section** | $\sigma_h$ $(cm^2)$ | 1E-15 |

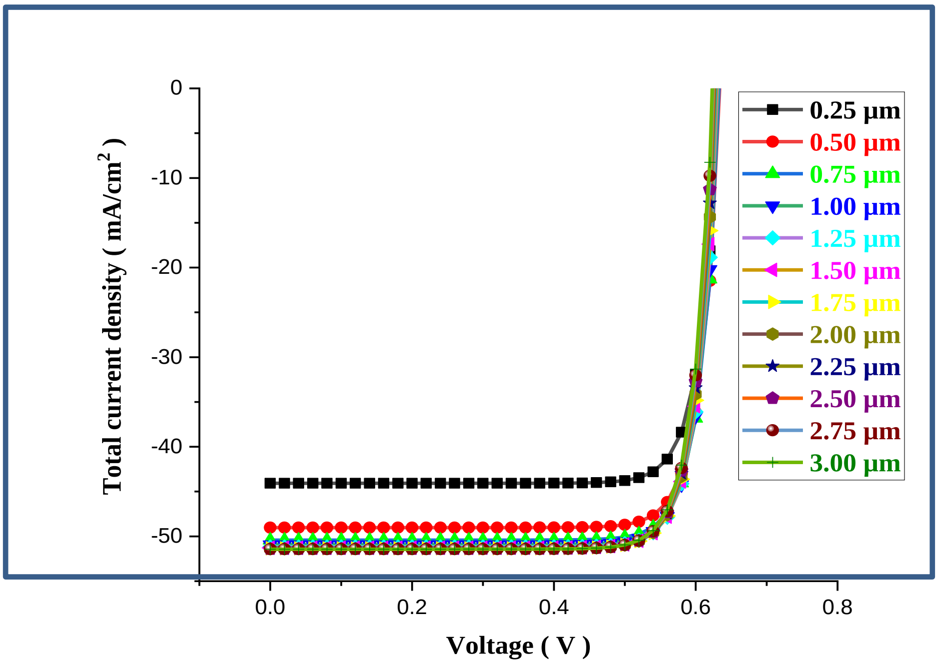

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**Figure (2) Effect of the Thickness of the p-CCZTSe apsorption layer on the (I-V) curve .**

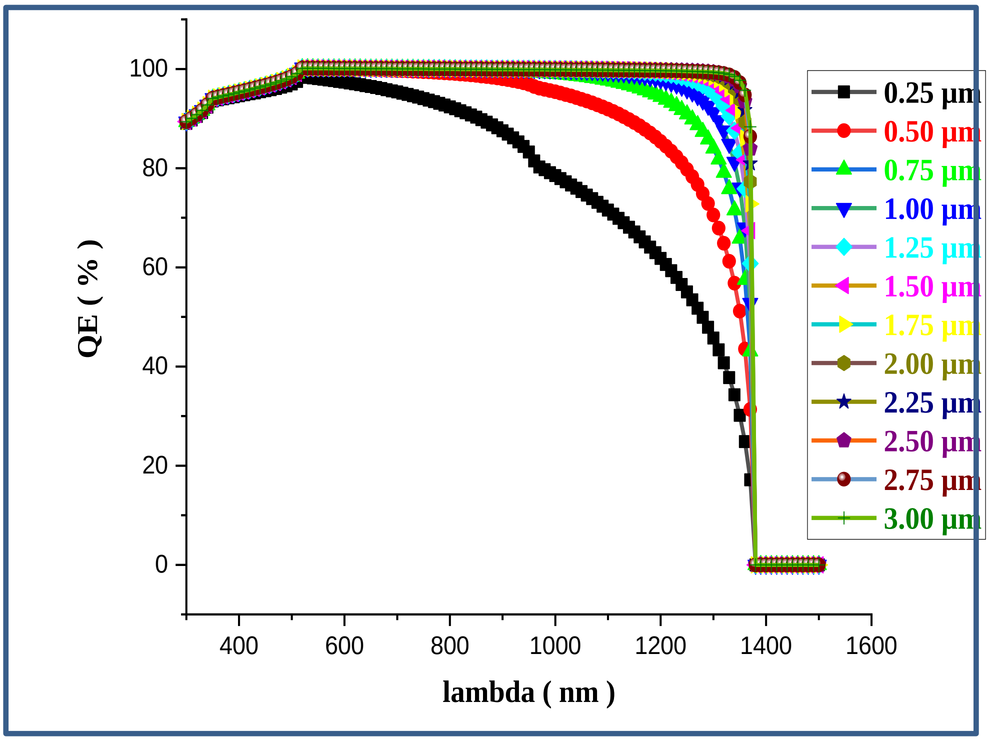


**Figure (3) Effect of Thickness on Quantum-efficiency (QE) Curve.**

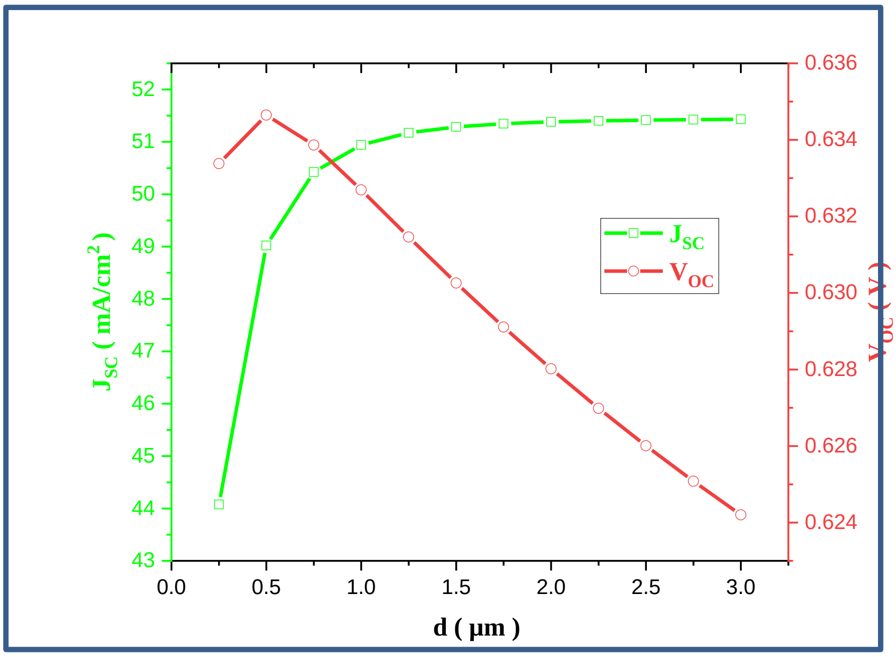


**Figure (4) Effect of the Thickness of the p-CCZTSe absorption layer on the open circuit voltage ($V_{OC}$) and current density ($J_{SC}$) .**

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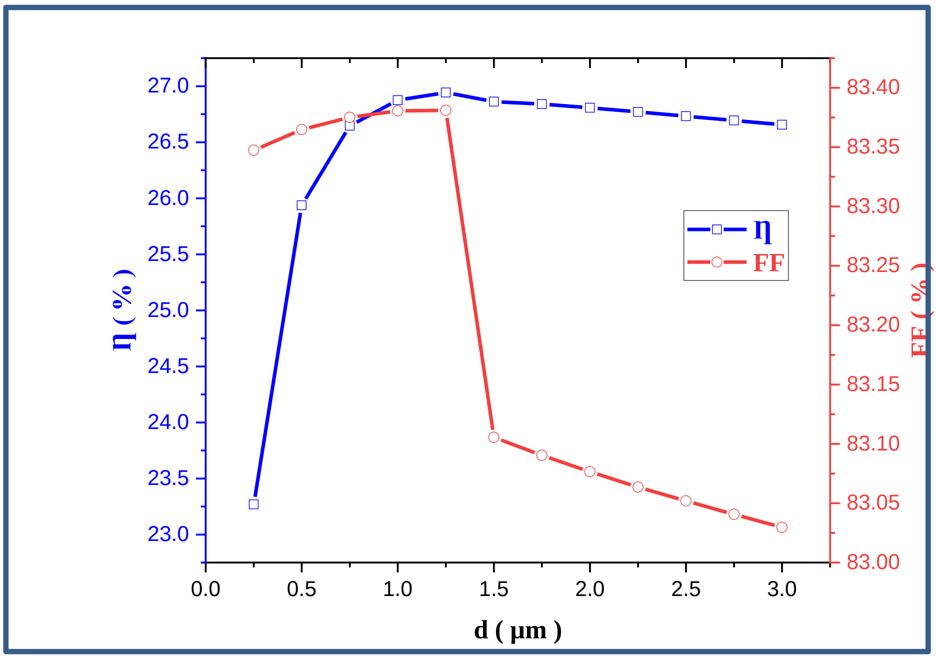
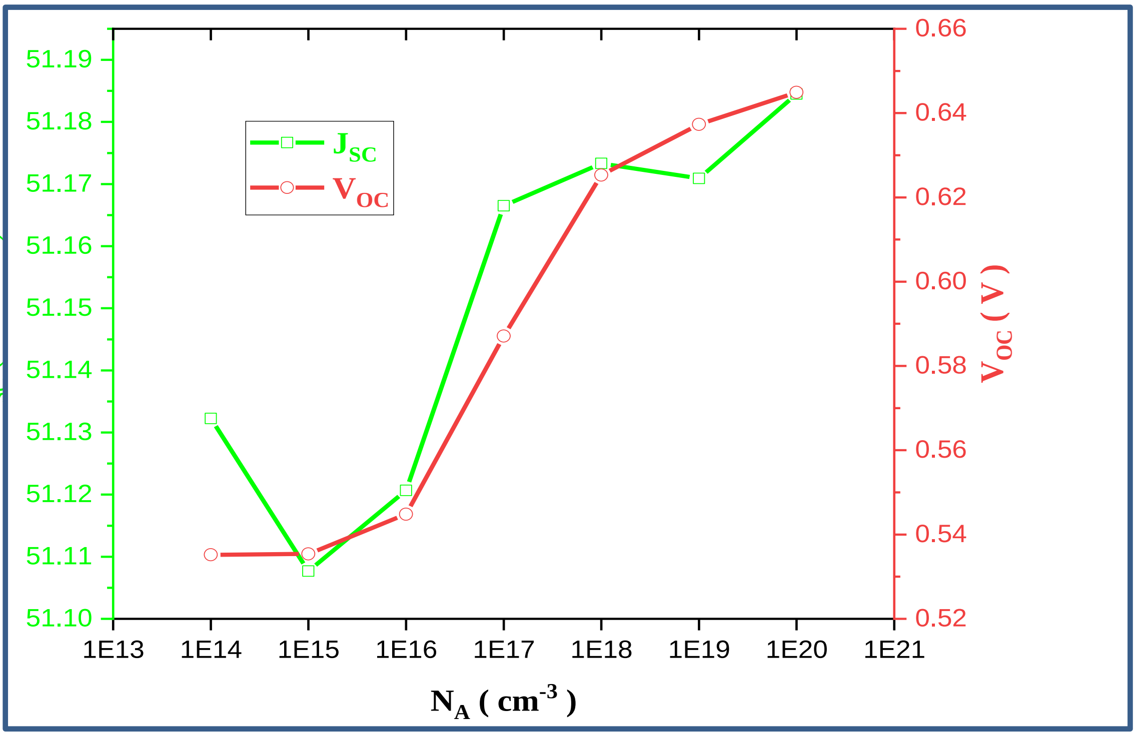



**Figure (5) Effect of the Thickness of the p-CCZTSe absorption layer on the efficiency value (Ƞ) and fill factor (FF) .**

**2-Effect of Acceptor Concentration**

The concentration of the receptors ($N_A$) in the absorption layer was changed from 1E14- 1E20cm$^{-3}$ with the thickness fixed at 1.25 µm. Figure (6) shows the effect upon ($V_{OC}$) and ($J_{SC}$) while Figure (7) shows the effect upon efficiency (η) and Fill-Factor (FF). $V_{OC}$ increases from 0.535V at $N_A$= 1E14 cm$^{-3}$, up to 0.644V at $N_A$=1E20 cm$^{-3}$. The change in ($J_{SC}$) generally is small. The efficiency increases from 19.68% up to 27.59% and( FF) increases from 71.91- 83.58% in the same range of change in $N_A$ as above. The main reason behind this is that as the concentration of the acceptors increases, the saturation current of the device increases, and then the ($V_{OC}$)increases as a result of which photons of longer wavelength and having less energy are absorbed deeper in the (CCZTSe)- absorption layer. Therefore, the conversion efficiency is highly dependent on the effect of acceptor concentration [21]. As it is clear from Figure 7, the efficiency (Ƞ) and fill factor (FF) improves.




**Figure(6): Effect of Acceptor Concentration in the absorption layer on the current density($J_{SC}$)and open circuit voltage ($V_{OC}$)**

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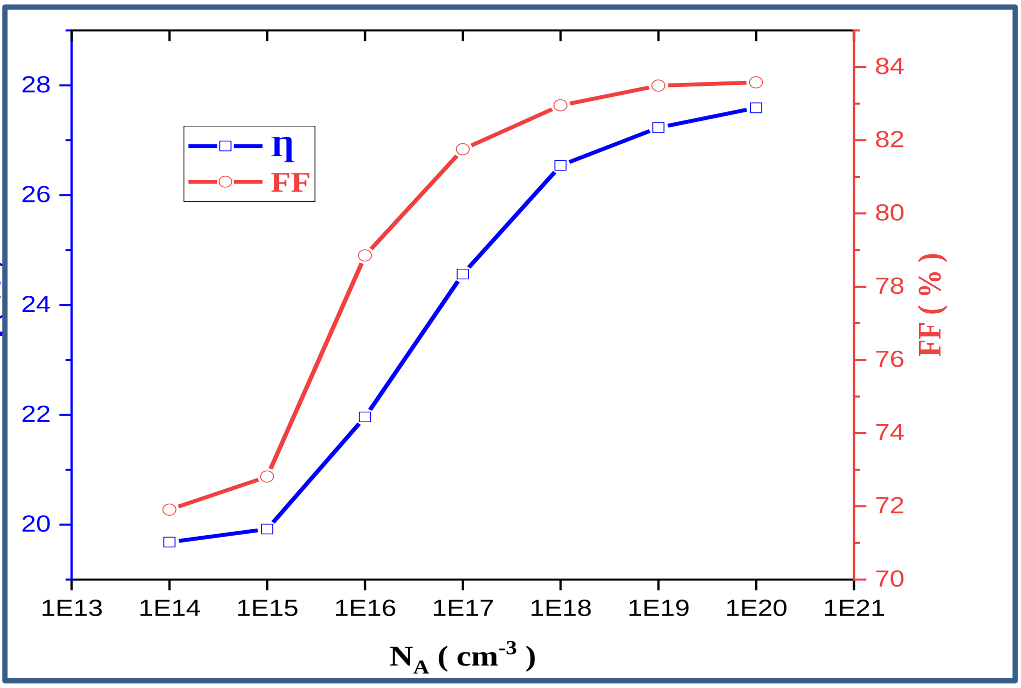


**Figure (7): Effect of Acceptor Concentration in the absorption layer on cell efficiency (η) and filling factor (FF)**

**3-Effect of Donor Concentration**

The concentration donors in the n-CdS buffer layer was changed from 1E14- 1E20 $cm^{-3}$, the thickness and acceptor-concentration of the absorbent layer was kept constant at 1.25 µm and 1E18 $cm^{-3}$. The change in ($V_{OC}$) and ($J_{SC}$) are minor as shown in Figure (8). Similarly, the change in the conversion-efficiency (η) is negligible as shown in Figure (9). The filling factor (FF) remains almost constant at about 82.95% up to 1E17 $cm^{-3}$, as shown in Figure 9.

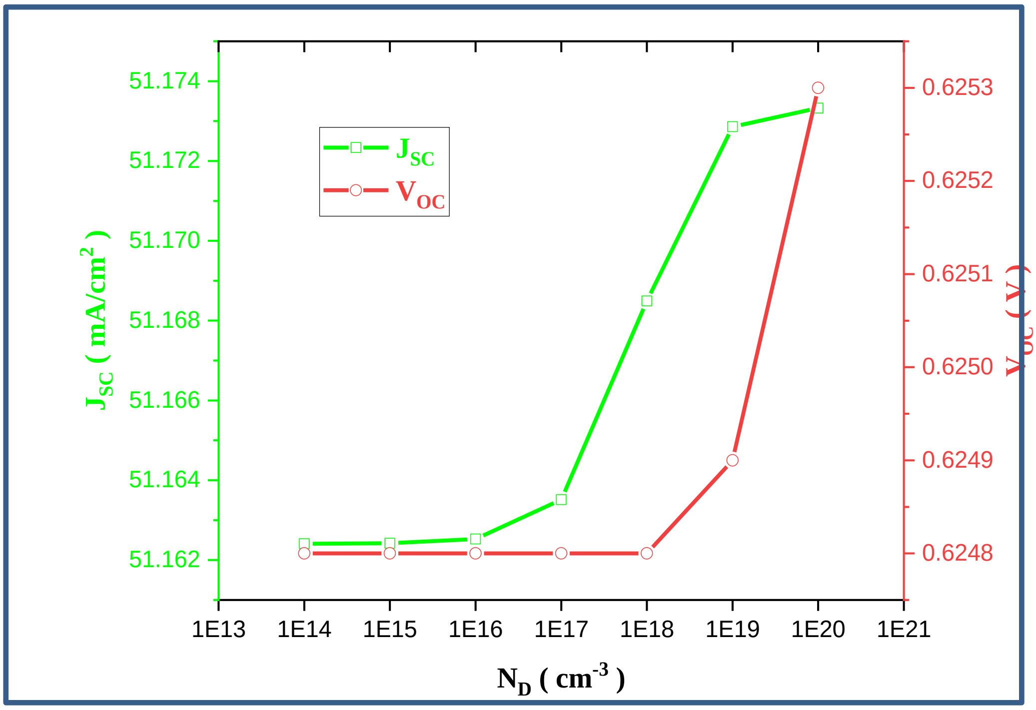


**Figure (8): Effect of donor concentration ( $N_D$ ) in the n-CdS layer on ($J_{SC}$) and ($V_{OC}$)**

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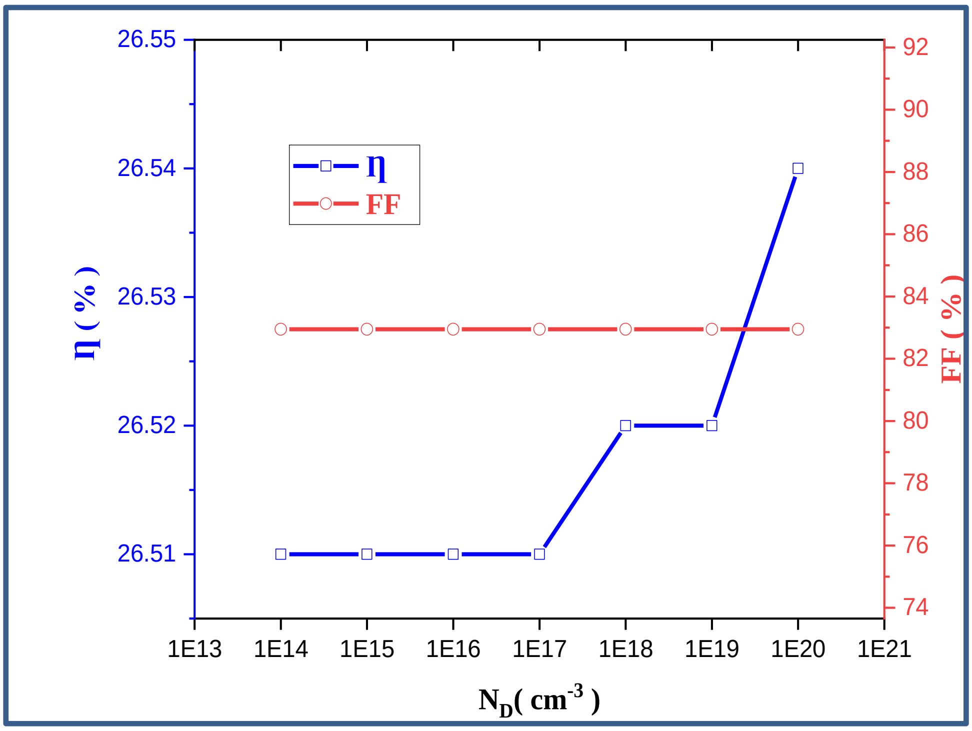


**Figure (9): Effect of the donor concentration ($N_D$) in the n-CdS layer on the cell efficiency (η) and the filling factor (FF).**

**4-Effect of defects density in the absorbent layer**

The effect of the defects on the p-CCZTSe absorption layer was investigated in the concentration range from 1E13 - 1E17 $cm^{-3}$, while keeping the thickness and the acceptor-concentration at 1.25 µm, and 1E18 $cm^{-3}$ respectively. The donor-concentration in the CdS- layer was fixed at 1E20 $cm^{-3}$. Figure (10) shows the I-V curves for various defect-densities. Both $V_{OC}$, and $J_{SC}$ decrease with increasing density of defects in the absorbent layer, which is made clear in Figure (11). The numerical values are given in Table (6). The reduction in the value of ($V_{OC}$, $J_{SC}$) may be due to increased trapping centers for minority carriers and thus increases the recombination rate and hence reduces the value of the open circuit voltage**.** This is due to the process of recombination in the material and the surfaces of the semiconductor [22].

From Table (6), the efficiency value decreases from (27.27%) at a defect-density (1E13 $cm^{-3}$) to (13.05%) at (1E17 $cm^{-3}$), which is shown also in Figure (12). The value of the fill factor (FF) is reduced from (83.54%) at a defect-density of (1E13 $cm^{-3}$) to (69.99%) at (1E17 $cm^{-3}$), which is also displayed in the Figure (12). The reduction of the open circuit voltage and filling factor leads to a decrease in the efficiency value as in Equation (4)[23]. And this is due to the presence of the recombination current in the depletion region and due to the increase in the process of recombination at the interface [14]. The Quantum-efficiency (QE) is (88.21 %) at the defect-density (1E13$cm^{-3}$), it decreases to (84.55 %) when the defects-density increases to (1E17$cm^{-3}$) as shown in Figure (13). This is due to the recombination process at the back surface and a decrease in the level of absorption of photons at long wavelengths and short carrier propagation lengths.

**Table (3) Cell properties when changing the defect density ($N_{def}$) in the p- CCZTSe absorbent layer**

| $N_{def}$ $cm^{-3}$ | $V_{OC}$ V | $J_{SC}$ $mA/cm^2$ | FF % | η % |
|---|---|---|---|---|
| **1E13** | 0.6375 | 51.207513 | 83.54 | 27.27 |
| **1E14** | 0.6253 | 51.173324 | 82.95 | 26.54 |
| **1E15** | 0.5843 | 50.842849 | 81.17 | 24.11 |
| **1E16** | 0.5254 | 48.365008 | 77.28 | 19.64 |
| **1E17** | 0.4516 | 41.273569 | 69.99 | 13.05 |

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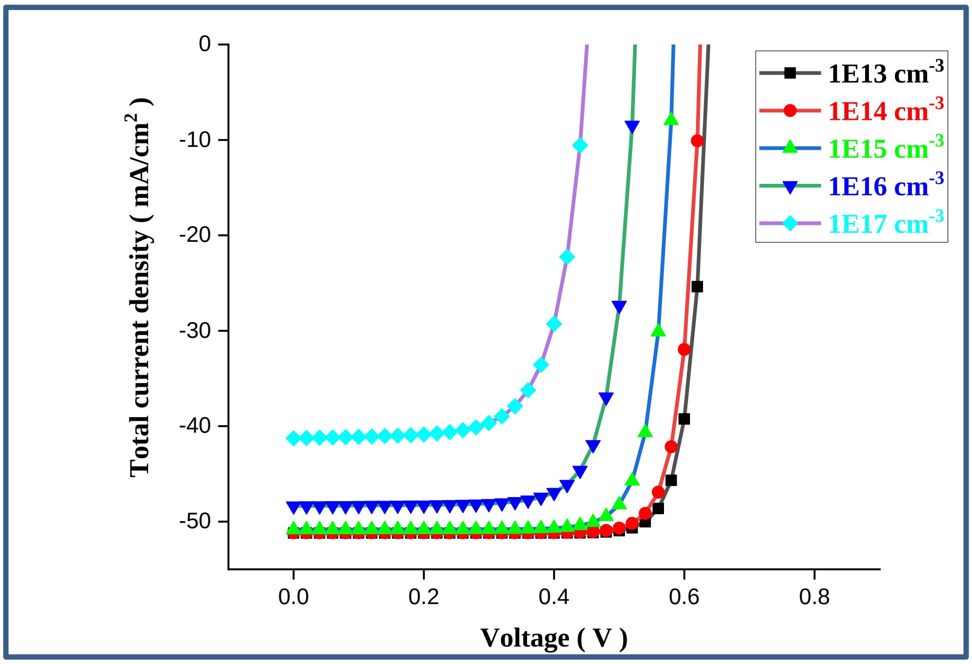


**Figure (10) Effect of defect density in p-CCZTSe absorption layer on the I-V curve**

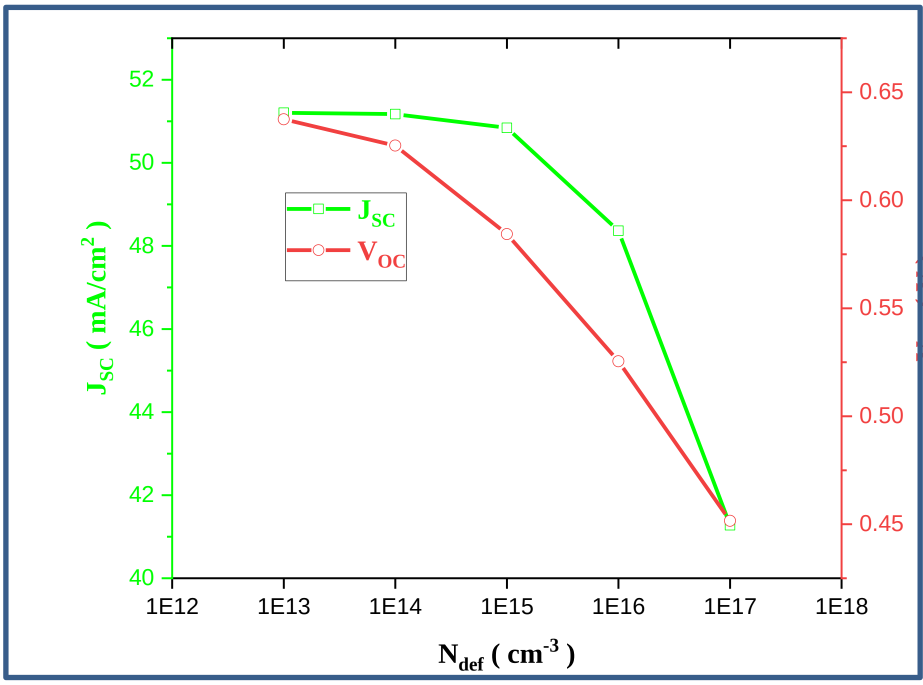


**Figure (11) Effect of the defect density in the p-CCZTSe absorption layer on $V_{OC}$ and $J_{SC}$.**

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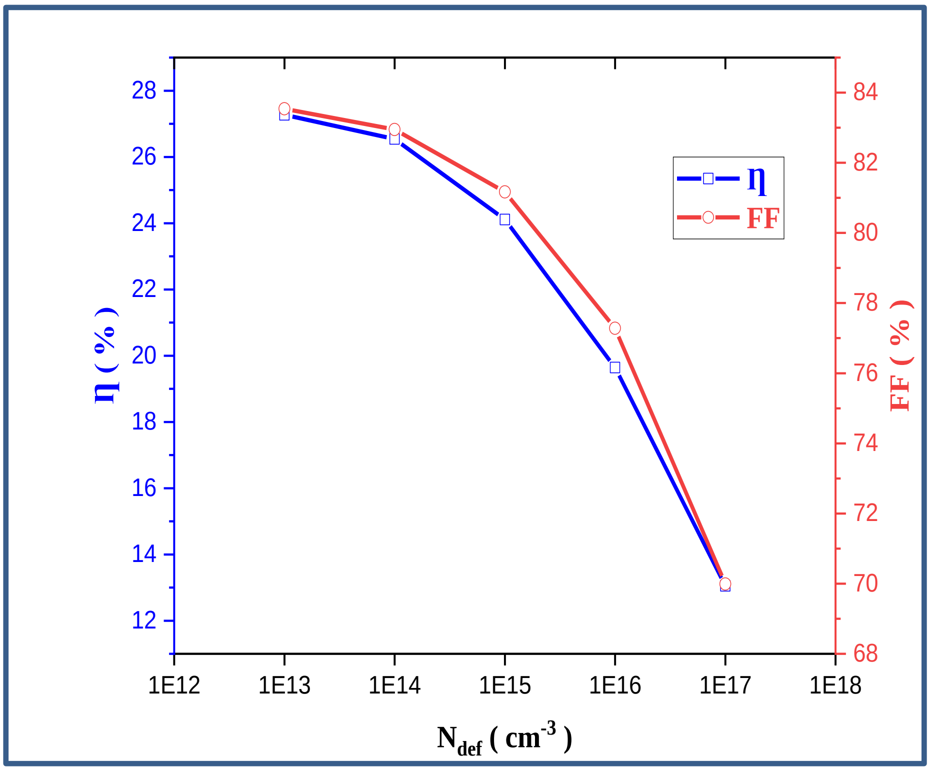


**Figure (12): Effect of the defect density of the p-CCZTSe adsorption layer on the efficiency value (η) and fill factor (FF)**

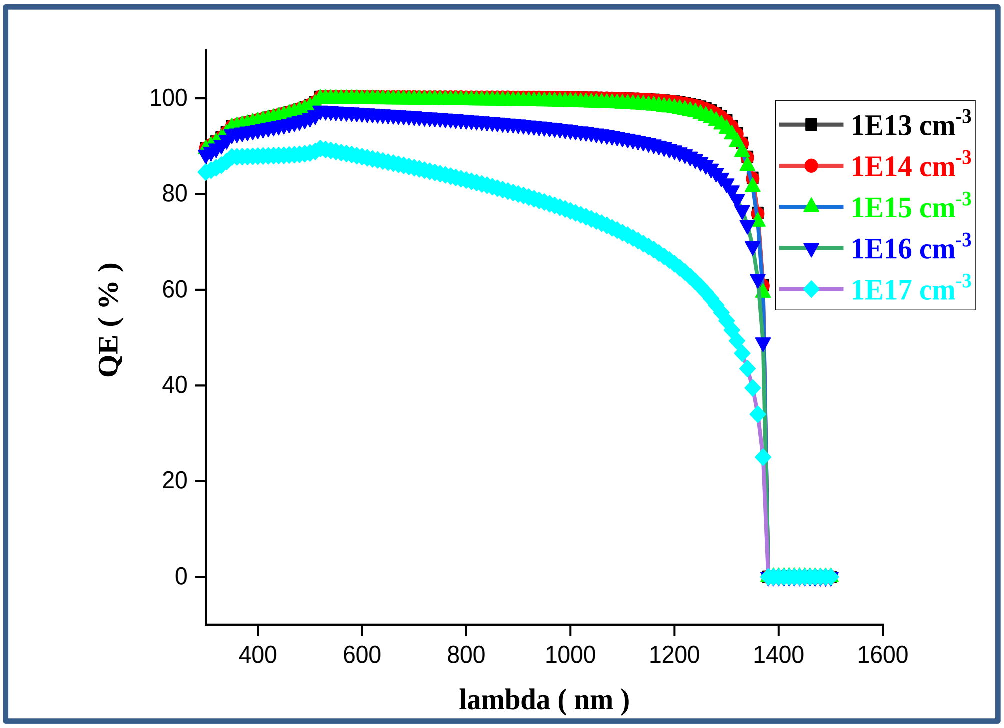


**Figure (13) Effect of defect density (Ndef) on the Quantum efficiency (QE)**

**Conclusions:**

From the simulation process, using SCAPS-1D software, it was found that changing the thickness of the (CCZTSe)-absorbent layer from 0.25- 3μm results in an increase in the conversion-efficiency (η), from 23.27% to 26.66% with a maximum of 26.94% at a thickness of 1.25 μm, and an increase in short-circuit current density ($J_{SC}$) from 44 - 51.4 mA/$cm^2$. The fill-factor (FF), and the open-circuit voltage ($V_{OC}$) remains almost constant at about 83% and 0.63 V respectively. Increasing the defects-

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density ($N_{def}$ ) from 1E13 - 1E17 cm$^{-3}$, in the (CCZTSe)- absorption layer leads to a decrease in the efficiency from 27.27% to 13%. The FF decreases from 83.5% to about 70%, the short-circuit current density ($J_{SC}$) decreases from 51 - 41 mA/cm$^2$. the open-circuit voltage ($V_{OC}$) decreases from about 0.64 V to about 0.45 V. And we notice an improvement in efficiency (η), (FF), and ($V_{OC}$) when increasing the concentration of the acceptors ($N_A$) in the (CCZTSe)- absorption layer in the range (1E14-1E20cm$^{-3}$). The efficiency (η), increases from about 19.7% to about 27.6%, FF increases from 72% to 83.6% and ($V_{OC}$) increases from 0.53 - 0.64 V, while ($J_{SC}$) remains almost constant. No change produced when we changed the donor-density ($N_D$) in the CdS buffer layer.

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